Pentanamide, N-(3-nitrophenyl)-

Inchi: InChI=1S/C11H14N2O3/c1-2-3-7-11(14)12-9-5-4-6-10(8-9)13(15)16/h4-6,8H,2-3,7H2,1H
InchiKey: UYUWKCAOJYPGIZ-UHFFFAOYSA-N
Formula: C11H14N2O3
SMILES: CCCCC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
gf	140.54	kJ/mol	Joback Method
hf	-115.18	kJ/mol	Joback Method
hfus	35.96	kJ/mol	Joback Method
hvap	72.79	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.723		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	2073.00		NIST Webbook
tb	738.62	K	Joback Method
tc	972.33	K	Joback Method
tf	498.87	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.40	J/mol×K	738.62	Joback Method
cpg	482.91	J/mol×K	777.57	Joback Method
cpg	494.45	J/mol×K	816.52	Joback Method
cpg	505.08	J/mol×K	855.48	Joback Method
cpg	514.85	J/mol×K	894.43	Joback Method
cpg	523.81	J/mol×K	933.38	Joback Method
cpg	532.01	J/mol×K	972.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306896&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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